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SLIP ALONG A BOUNDARY FORMING AN INCOMMENSURABLE

STRUCTURE

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UDC 539.219.3

The boundary dividing a plane with rational indices, for example, (100) and (110) in a cubic lattice, is considered. The planes are oriented so that the direction [001] is common. Then the interatomic distances are incommensurable in the perpendicular direction. The conditions of thermal activation slip along such a boundary are studied. For sufficiently small stresses the dependence of the derivative of the slip velocity on the stress has a discontinuous nature.

Comparatively great attention has been paid to the thermodynamic properties of physical systems forming incommensurable structures [1], while the kinetic phenomena of the rearrangement of an incommensurable structure under the influence of external forces have been discussed much less in the literature. In particular, the slip of the crystals on whose interface an incommensurable atomic structure forms is one of these forces.

In this report we confine ourselves to the case of one-dimensional incommensurability, when the interatomic distances are incommensurable in the boundary plane in the τ direction, but are commensurable in the perpendicular direction in the boundary plane. Such a boundary can be both interphase and intergranular. A boundary at which the faces (100) and (110) adjoin crystals with cubic structures can serve as an example.

We denote the crystallite periods in the direction of τ by a_1 and a_2 . In the above the crystallographic directions [010] and [110] of adjacent crystallites are located along τ , while the direction [001] is common to them. Then $a_1 = a$, $a_2 = a\sqrt{2}$, where a is the lattice constant.

We first consider the geometric pattern of the superpositions in the boundary plane. The positions of the atomic sites in the aggregate form a vernier in the τ direction. We denote by ξ the displacement (distance) between two atoms of neighboring crystallites in the τ direction. It is characteristic of incommensurable periods that all ξ will be different and equally probable. The value $\xi = 0$ will be satisfied for only one pair of atoms.

We introduce the density function $n(\xi)$ of the distribution over ξ . We plot the atomic sites of one crystallite in the τ direction along the x axis, and the other along the y axis. Then the plane is covered by a rectangular lattice of points, each of which corresponds to a pair of sites. The distance ξ between the pair of sites of the incommensurable structure will be equal to the section of a straight line, parallel to the y axis and enclosed between the point corresponding to this pair of sites and the bisector $y = x$. If we now construct the straight lines $y - x = \xi$ and $y - x = \xi + \Delta\xi$, the number of points per unit length which are between these straight lines is equal to the number of atoms with distances from ξ to $\xi + \Delta\xi$, equal to $n(\xi)\Delta\xi$. Evidently, the point density is expressed in the form

$$n(\xi) = 1/a_1 a_2. \quad (1)$$

The relative displacement $\Delta\xi$ of the crystallites along the boundary will be accompanied by coincidences of the positions of the atomic sites of neighboring crystallites at certain

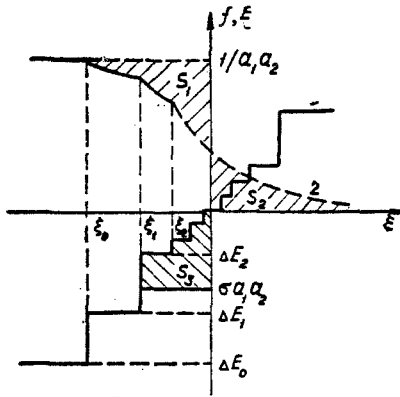


Fig. 1. The dependence of the energy on the distance ξ (1) and the distribution function with respect to ξ (2).

times. The number ΔN of such coincidences per unit length of the incommensurable structure is

$$\Delta N = n \Delta \xi. \quad (2)$$

Therefore, the relative displacements of the crystallites, taken over ΔN coincidences per unit length of the incommensurable structure, is

$$\Delta \xi = \Delta N a_1 a_2. \quad (3)$$

If dislocation representations are used, $\Delta \xi$ denotes the displacement of the crystal due to the shift of the dislocations with the Burgers vector a_1 , distributed in the slip plane with linear density ΔN , by a_2 . The relative displacement of the crystallites B in the case of a single migration per unit length ($\Delta N = 1$) is $B = a_1 a_2$.

For the consideration of the actual pattern of the atomic motion in the case of the relative displacements of the crystallites the interaction of the atoms in the contact region must be taken into account. The lower crystal can be replaced by the periodic potential field in which the atoms of the upper crystal move. We will assume for simplicity that one symmetric peak and well occurs for each period of the potential field. We consider an atom which is exactly on the peak of the potential relief. For the convenience of the subsequent discussion we assign the distance $\xi = 0$ to this atom, this corresponding to the displacement of the origin of the distance by half of the period of the potential relief. The position of the atom on the peak corresponds to unstable equilibrium.

This statement is obvious when the interaction of the atoms on different sides of the boundary is greater than in the boundary plane. In the other limiting case for the establishment of the fact of instability we can use the representations of the pinning of a soliton on a crystal lattice developed in [2], where it is shown that the pinning energy of the soliton decreases exponentially as the interaction between the atoms of neighboring lattices decreases, but does not vanish. Therefore, the atom which is exactly on the peak of the potential relief slides into one of two symmetrically positioned potential wells.

If the two superimposed lattices are shifted so that the atom which was previously on the peak is displaced from it by the small distance ξ , the curve of the potential energy as a function of the deviation of the atom from a certain mean position becomes asymmetric with a deeper potential well in the direction of displacement ξ . For small ξ , together with the continuous increase in the difference $\Delta E(\xi)$ between the two minimum energies there is, correspondingly, also an abrupt change. This last is due to the migrations of the atoms in the other sections of the incommensurable structure into deeper potential wells similar to that considered. Since such transitions are equivalent to the formation of a dislocation dipole with the dipole moment per unit length $a_1 a_2$, they lead to the development of the stresses $\sigma^{(i)} \approx \mu a_1 a_2 / r^2$, where μ is the shear modulus, r is the distance between the two interacting atomic configurations.

At the same time, ΔE changes by a jump to

$$\Delta E = \sigma^{(i)} a_1 a_2 \approx \mu a_1^2 a_2^2 / r^2.$$

The functional dependence $r(\xi)$ which indicates the sequence of coincidences of the positions of the atoms when the crystals are displaced represents one of the variants of the "devil's staircases" [1, 3] (see Fig. 1). Below we discuss the relatively high jumps of ΔE which arise on the migration of adjacent atoms.

Under conditions of static equilibrium it is evident that the right-hand wells are occupied for positive ξ ($\xi \ll a_1, a_2$) and the left-hand wells are occupied for negative ξ . After the application of external stresses a further difference in the levels of the energy minima appears, so that $\Delta E(\xi) \rightarrow \Delta E(\xi) + \sigma a_1 a_2$, as a result of which a thermal fluctuation transition into a lower potential well starts to occur.

We will assume that the transition of the atomic row from one well into the other starts from the origin of a double kink, as this occurs at the dislocation. Then for the time of transition of the atomic row from one well into the other in the case of small σ the following expression can be written [4]:

$$\tau = A/(\sigma a_1 a_2 + \Delta E(\xi)). \quad (4)$$

The energy of the kink E_0 appears in the coefficient A [4]. Here $\Delta E(\xi)$ is the difference between the bottoms of the left-hand and right-hand wells.

In the initial period the slip velocity of the crystallites is determined by the transitions which have the finite time τ . The boundary of the region of the values of ξ for which the transitions are accomplished is determined from the conditions

$$\Delta E(\xi) = -\sigma a_1 a_2. \quad (5)$$

Therefore, the initial velocity

$$v = \int_{\xi_1}^0 \frac{d\xi}{\tau(\xi)} = \frac{1}{A} \int_{\xi_1}^0 (\Delta E(\xi) + \sigma a_1 a_2) d\xi. \quad (6)$$

Thus, the initial velocity is determined by the hatched area S_3 in Fig. 1. The increase in the stress within one step leads to a linear increase in the initial velocity:

$$v = v_0 + \eta \sigma, \quad v_0 = \frac{1}{A} \int_{\xi_1}^0 \Delta E(\xi) d\xi, \quad \eta = |\xi_1|/A. \quad (7)$$

On the transition to a new step with an increase in σ the proportionality factor changes by a jump to $\Delta\eta = |\xi_2 - \xi_1|/A$.

On the expiration of the time of adjustment after the application of the external stress a structure which belongs to the category of dissipative structures [5] and which remains the same during the subsequent slip is established in the incommensurable system.

We introduce the probability $f(\xi, t)$ that the atom is in the left-hand well. Under non-equilibrium conditions the following kinetic equation can be written down for the function f :

$$\dot{f} = -f/\tau. \quad (8)$$

Here the relaxation time τ depends not only on ξ but also on the rearrangements of the neighbors which reflect the correlation effects in the case of motion. Assuming, however, that τ is determined by the initial distribution in the incommensurable system, it being possible to consider this as the first step of an iteration process, then setting $f(\xi, t) = f(\xi + vt)$, this corresponding to a steady process, we obtain

$$f \tau + v \frac{\partial f}{\partial \xi} = 0. \quad (9)$$

Let an external stress be applied such that

$$\Delta E_2 < \sigma a_1 a_2. \quad (10)$$

ΔE_1 and ΔE_2 are shown in Fig. 1. The solution of (9) is expressed in the form

$$f(\xi) = \exp\left(-\int_{\xi_1}^{\xi} \frac{d\xi'}{v\tau}\right). \quad (11)$$

We find the slip velocity v , which appears as a parameter in (11), from the condition

$$-\xi_1 = \int_{\xi_1}^{\infty} f(\xi) d\xi, \quad (12)$$

which corresponds to the satisfaction of the equality of the areas S_1 and S_2 , hatched in Fig. 1.

In expression (11) τ changes abruptly on the transition from one step to another, in accordance with (5). Thus, the distribution function on the transition from one step to another is continuous with a bend at $\sigma = \Delta E_1/a_1a_2$.

We substitute (11) in (12) and differentiate the two sides of the obtained equation with respect to v . After certain manipulations and the use of the relations $d\tau/dv = (d\tau/d\sigma)/(d\sigma/dv)$ we obtain

$$\eta = \frac{dv}{d\sigma} = \frac{a_1a_2}{AJ_1} \int_{\xi_1}^{\infty} (\xi - \xi_1) \exp\left(-\int_{\xi_1}^{\xi} \frac{d\xi'}{v\tau}\right) d\xi. \quad (13)$$

Here

$$J_i = \int_{\xi_i}^{\infty} \exp\left(-\int_{\xi_i}^{\xi} \frac{d\xi''}{v\tau}\right) \int_{\xi_i}^{\xi} \frac{d\xi'}{v\tau} d\xi. \quad (14)$$

The superscript of ξ in (14) indicates the lowest step from which the transitions are accomplished.

Now let the external stress increase so that condition (10) is replaced by the condition

$$\Delta E_1 < \sigma a_1a_2 < \Delta E_0. \quad (15)$$

Then both $f(\xi)$ and $dv/d\sigma$ are expressed by the same equations (11) and (13), only we have the subscript 0, and not 1. We find the jump in the derivative of the velocity with respect to the stress, $\Delta\eta$, on the transition from the first to the zeroth step. It is simplest of all to trace the change in $dv/d\sigma$ at the time of transition from one step to another if the integrals in the numerator and denominator of (13) are represented in the form

$$\int_{\xi_0}^{\infty} \{\dots\} d\xi = \int_{\xi_0}^{\xi_1} \{\dots\} d\xi + \int_{\xi_1}^{\infty} \{\dots\} d\xi. \quad (16)$$

Then after certain transformations we obtain

$$\Delta\eta = a_1a_2 (\xi_0 + \xi_1) (\xi_0 - \xi_1) / 2AJ_0. \quad (17)$$

Carrying out a rough estimate of the integral J_0 , we find $J_0 \sim v\tau \sim |\xi_0|$. Thus, the jump in the viscosity on the transition to the next step is equal in order of magnitude to a similar jump at the initial velocity.

In conclusion we note that the functions $v(\sigma)$ obtained are due to two factors: the dependences of the mobility of the dislocation dipoles and their number on the external stresses. The relative slip of the crystallites which form an incommensurable structure at the joining point is realized rapidly by means of the thermally activated migration of the atoms in the two-well configurations with the simultaneous preparation of such configurations at new surface points. At the same time, the relative slip for one of the periods is realized by means of one migration of each of the atoms of the corresponding lattice. The mean distance a_1a_2/ξ between the atomic configurations which participate in the parallel process of rearrangement decreases as the stress increases, in accordance with Fig. 1.

The authors are grateful to V. E. Egorushkin for his discussion of the present paper.

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